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REAL TIME NEURAL NETWORK RAMAN SIGNAL ENHANCEMENT

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ABSTRACT

A Raman spectrometer is being developed that utilizes Neural Network (NN) signal processing to extract the chemical signatures of VOCs from spectra exhibiting extremely high noise levels, resulting in enhanced sensitivity of the Raman technique. The Raman system is used to both identify and quantify DOE/DOD target organic and inorganic contaminants in both solid samples (Hanford UST) and ground-water, with a secondary application being the location and identification of subsurface NAPLs. The system utilizes a NN package that is being developed by Physical Optics Corporation (POC) for real-time signal extraction from high background noise in conjunction with a remote Raman spectrometer being developed at LLNL. The POC NN is unique in that it is based on a hardware rather than a software approach. The advantages of the hardware approach are the large number of data points that can be simultaneously analyzed and greatly reduced processing time. The NN is trained to recognize chemical contaminants at concentration levels potentially ranging from EPA limits in soils and water to neat solids and liquids.

The NN has been trained to recognize the Raman spectral signatures of the organochlorides CCl_4, $CHCl_3$, DCM, TCE, and TCA. The training of the NN is accomplished using single component organochloride spectra with signal to noise ratios in the range of 5:1 to 35:1. Once the training is complete, the NN is asked to identify approximately 75 low S/N (<1:1) spectra of individual organochlorides and four and five component organochloride mixtures. The NN gives correct identifications with 93+% accuracy, and gives 100% rejection of spectra consisting only of noise. Only *30 milliseconds* are required to perform a complete deconvolution of 1024 spectral data points, including composition identification and notification of the operator as to the results. The NN is also able to positively identify 2500 ppm (V/V) CCl_4 in methanol with 100% confidence and 250 ppm (V/V) with 65% confidence. This represents an enhancement of the detection limits of CCl_4 by Raman spectroscopy by 2 orders of magnitude. These results indicate the power of the NN system to both extract real signal which appeared nonexistent from extremely high noise levels and readily provide component analysis of highly complex spectral information. We are continuing to develop the potential of the NN into a viable system that has a wide application in analytical chemistry.

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